Ethyl phenylacetate

101-97-3 | DTXSID6044353

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 5.89

Global applicability domain: Inside

Local applicability domain index: 5.84e-01

Confidence level: 5.93e-01

Nearest Neighbors from the Training Set

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O,O-Diethyl dithiophosphate
Measured: 5.01
Predicted: 5.43

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Isophorone
Measured: 2.00
Predicted: 3.19

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Triallylamine
Measured: 3.55
Predicted: 4.23

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N,N-Dimethyl-1,2-dithiolan-4-amine
Measured: 52.5
Predicted: 17.5

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Triethylamine
Measured: 4.90
Predicted: 5.95